Study offers new insights into understanding and controlling tunneling dynamics in complex molecules

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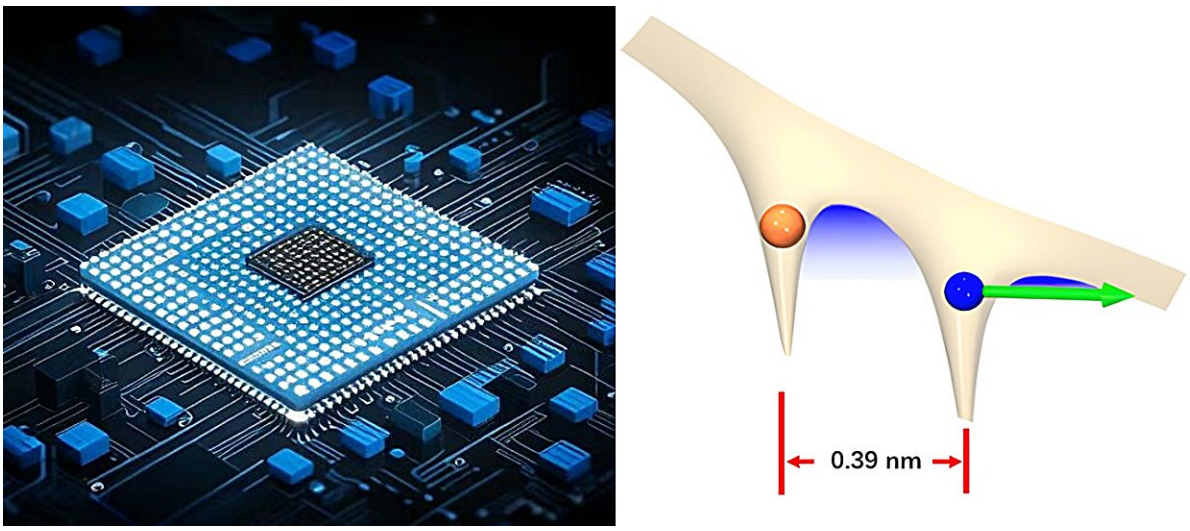


The electronic chip and the Van der Waals complex with an internuclear distance 0.39 nm. Credit: Ming Zhu, Jihong Tong, Xiwang Liu, Weifeng Yang, Xiaochun Gong, Wenyu Jiang, Peifen Lu, Hui Li, Xiaohong Song & Jian Wu

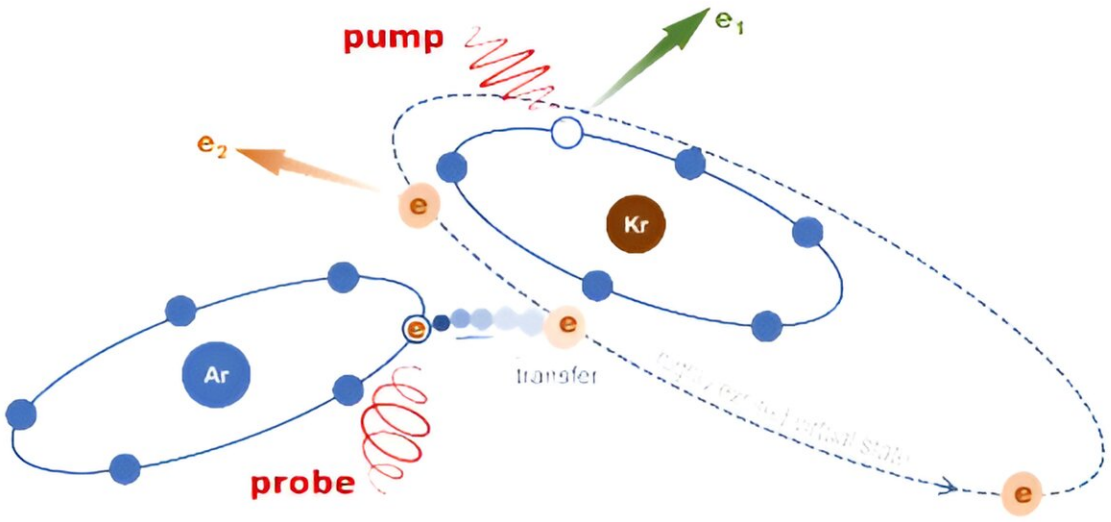
Tunneling is one of most fundamental processes in quantum mechanics, where the wave packet could traverse a classically insurmountable energy barrier with a certain probability.

On the atomic scale, tunneling effects play an important role in molecular biology, such as accelerating enzyme catalysis, prompting

spontaneous mutations in DNA and triggering olfactory signaling cascades.

Photoelectron tunneling is a key process in light-induced chemical reactions, charge and energy transfer and radiation emission. The size of optoelectronic chips and other devices has been close to the sub-nanometer atomic scale, and the quantum tunneling effects between different channels would be significantly enhanced.

The real-time imaging of electron tunneling dynamics in complex molecules has important scientific significance for promoting the development of tunneling transistors and ultrafast optoelectronic devices. The effect of neighboring atom on electron tunneling dynamics in complex molecules is one of the key scientific issues in the fields of quantum physics, quantum chemistry, nanoelectronics, etc.



The electron emitted from Ar atom is firstly trapped to the highly excited transient states of the Ar-Kr^+ before its eventual releasing to the continuum. A

linearly polarized pump laser pulse is used to prepare the Ar-Kr^+ ion by removing *e*1 from Kr site, and a time delayed elliptically polarized probe laser pulse is used to track the electron transfer mediated electron tunnelling dynamics (e2, orange arrow). Credit: Ming Zhu, Jihong Tong, Xiwang Liu, Weifeng Yang, Xiaochun Gong, Wenyu Jiang, Peifen Lu, Hui Li, Xiaohong Song & Jian Wu

In a paper published in *Light: Science & Applications*, a team of scientists from Hainan University and East China Normal University designed a van der Waals complex Ar-Kr^+ as a prototype system with an internuclear distance of 0.39 nm to track the electron tunneling via the neighboring atom in the system of sub-nanometer scale.

The intrinsic electron localization of the highest occupied molecular orbital of Ar-Kr gives a preference of electron removal from Kr site in the first ionization step.

The site assisted electron hole in Ar-Kr^+ guarantees that the second electron is mainly removed from the Ar atom in the second ionization step, where the electron may straightly tunnel to continuum from the Ar atom or alternatively via the neighboring Kr^+ ionic core.

In combination with the improved Coulomb-corrected strong-field approximation (ICCSFA) method developed by the team, which is able to take into account the Coulomb interaction under the potential during tunneling, and by monitoring the photoelectron transverse momentum distribution to track the tunneling dynamics, it was discovered that there are two effects of strong capture and weak capture of tunneling electrons by neighboring atom.

This work successfully reveals the critical role of neighboring atom in electron tunneling in sub-nanometer complex systems. This discovery

provides a new way to deeply understand the key role of the Coulomb effect under the potential barrier in the electron tunneling dynamics, solid high harmonics generation, and lays a solid research foundation for probing and controlling the tunneling dynamics of complex biomolecules.

More information: Ming Zhu et al, Tunnelling of electrons via the neighboring atom, *Light: Science & Applications* (2024). DOI: 10.1038/s41377-023-01373-2

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